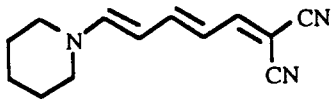
SUPPLEMENTARY MATERIAL FOR COMPOUND 1

1,1-dicyano-6-(1-piperidinyl)-1,3,5-hexatriene



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wps code	Pip-II-DCV
Name	1,1-dicyano-6-(1-piperidinyl)-1,3,5-hexatriene
Formula	$C_{13}H_{15}N_3$
Formula Weight	213.28
Crystal System	triclinic
Space Group	$P\bar{1}$
Cell Dimensions a, Å	5.332 (3)
b, Å	10.865 (3)
c, Å	11.790 (5)
α, °	72.25 (3)
β, °	79.41 (4)
γ, °	86.92 (3)
V, $Å^3$	639.4 (5)
Z	2
Density, calc, g cm^{-3}	1.11
Crystal color, habit	thin orange, parallelepiped
Crystal size, mm^3	0.07 x 0.09 x 0.21
μ, cm^{-1}	0.063
μ r_{max}	0.0132
maximum 2θ (scan type)	25°
range of h,k, l	-6-6, -12-12, -14-14
# of reflections measured	4551
# of independent reflections	2244
# reflections, $F_o^2 > 0$	1801
# reflections, $F_o^2 > 3\sigma(F_o^2)$	791
GOF, merge	???
R(merge) for refs meas. twice	0.081
secondary extinction (x 10^{-6})	0.9(4)
R, $F_o^2 > 0$	0.171
R, $F_o^2 > 3\sigma(F_o^2)$	0.077
GOF (number of parameters)	1.62, (1.46)
$(\Delta/\sigma)_{max}$ in final least squares	0.01
Final Difference map:	
Maximum, $eÅ^{-3}$	+ 0.42
Minimum, $eÅ^{-3}$	- 0.40

Data was collected at 294 K.
Hydrogen positions were assumed, C-H 0.95 Å, and repositioned once near the end of refinement.
Structure solved using MULTAN 88.

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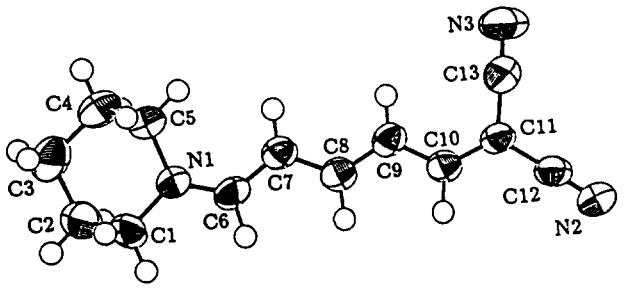

Figure 1

Schaefer, Tiemann and Marder

Figure 1: An ORTEP drawing of the molecule with 50% probability elipsoids showing the numbering system. Hydrogen atoms are drawn as circles of arbitrary small size.

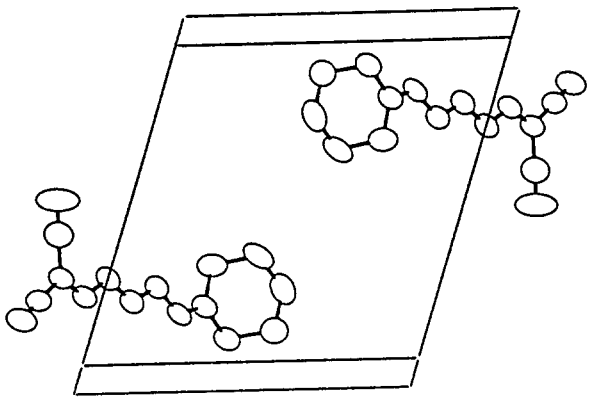

Figure 2.

Schaefer, Tiemann and Marder

Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Hydrogen atoms are not shown.

Table 1. Final Heavy Atom Parameters for 1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

x, y, z and U_{eq}[a] $\times 10^4$

Atom	x	y	z	U_{eq}
N1	2912(8)	3116(4)	2228(3)	652(12)
C1	1552(10)	4066(5)	1385(4)	761(16)
C2	1615(11)	5378(5)	1585(5)	873(18)
C3	434(12)	5267(6)	2886(6)	990(20)
C4	1887(12)	4262(6)	3747(5)	989(20)
C5	1872(10)	2984(5)	3503(4)	846(18)
C6	4811(10)	2427(5)	1870(4)	648(15)
C7	6269(10)	1517(5)	2540(4)	612(15)
C8	8225(10)	905(5)	1973(4)	625(14)
C9	9884(10)	1(5)	2519(4)	613(15)
C10	11787(10)	−533(5)	1851(4)	620(15)
C11	13653(9)	−1376(5)	2252(4)	580(15)
C12	15538(10)	−1837(5)	1451(4)	635(16)
N2	17041(9)	−2173(4)	779(4)	884(15)
C13	13805(10)	−1836(5)	3504(5)	772(18)
N3	13880(10)	−2165(6)	4504(4)	1251(22)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table 2. Heavy Atom Distances and Angles for 1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

	Distance(Å)		Angle(°)
N1 –C1	1.463(7)	C5 –N1 –C1	113.2(4)
N1 –C5	1.469(7)	C6 –N1 –C1	122.7(4)
N1 –C6	1.311(7)	C6 –N1 –C5	124.0(4)
C1 –C2	1.517(8)	C2 –C1 –N1	110.2(4)
C2 –C3	1.518(8)	C3 –C2 –C1	109.3(5)
C3 –C4	1.531(9)	C4 –C3 –C2	109.8(5)
C4 –C5	1.502(8)	C5 –C4 –C3	110.0(5)
C6 –C7	1.369(7)	C4 –C5 –N1	110.8(5)
C7 –C8	1.384(7)	C7 –C6 –N1	129.5(5)
C8 –C9	1.376(7)	C8 –C7 –C6	120.2(5)
C9 –C10	1.381(7)	C9 –C8 –C7	126.9(5)
C10 –C11	1.365(7)	C10 –C9 –C8	121.6(5)
C11 –C12	1.428(7)	C11 –C10 –C9	128.3(5)
C11 –C13	1.422(8)	C12 –C11 –C10	122.3(5)
C12 –N2	1.147(7)	C13 –C11 –C10	120.9(5)
C13 –N3	1.131(8)	C13 –C11 –C12	116.8(5)
		N2 –C12 –C11	177.9(6)
		N3 –C13 –C11	177.6(6)

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Table S1. Assigned Hydrogen Atom Parameters for 1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

x, y and $z \times 10^4$

Atom	x	y	z	B
H1A	−164	3792	1509	6.9
H1B	2357	4127	580	6.9
H2A	643	5976	1060	7.9
H2B	3315	5673	1421	7.9
H3A	−1293	5014	3038	9.0
H3B	547	6080	3021	9.0
H4A	1072	4166	4559	9.0
H4B	3590	4541	3634	9.0
H5A	171	2669	3685	7.6
H5B	2887	2386	3998	7.6
H6	5237	2580	1017	5.8
H7	5946	1309	3399	5.6
H8	8430	1129	1115	5.6
H9	9721	−258	3375	5.6
H10	11797	−280	1002	5.6

Table S2. Anisotropic Displacement Parameters for 1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N1	744(33)	741(33)	553(27)	149(27)	−188(24)	−296(24)
C1	965(46)	773(42)	710(37)	195(35)	−428(33)	−333(32)
C2	1113(50)	800(44)	762(40)	141(36)	−297(35)	−263(34)
C3	1274(57)	820(46)	1017(48)	116(41)	−150(43)	−532(39)
C4	1327(59)	1117(54)	750(42)	218(45)	−272(38)	−596(40)
C5	977(47)	963(47)	549(35)	215(36)	−71(31)	−228(33)
C6	779(44)	744(42)	561(33)	55(34)	−168(30)	−383(31)
C7	689(41)	653(39)	573(33)	5(33)	−144(30)	−281(31)
C8	703(41)	663(38)	619(33)	−35(32)	−205(30)	−297(30)
C9	649(41)	685(43)	609(35)	3(33)	−142(30)	−327(31)
C10	735(41)	680(39)	563(34)	6(32)	−218(30)	−301(30)
C11	601(39)	704(40)	478(32)	−10(32)	−108(28)	−233(29)
C12	767(44)	680(40)	485(33)	10(33)	−181(30)	−175(30)
N2	1084(42)	1044(39)	602(30)	284(32)	−194(28)	−381(28)
C13	716(42)	907(46)	680(39)	79(33)	−72(34)	−264(37)
N3	1194(47)	1904(60)	566(32)	306(39)	−194(30)	−268(36)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table S3. Complete Distances and Angles for 1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

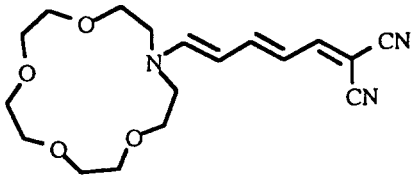
	Distance(Å)		Angle(°)
N1 –C1	1.463(7)	C5 –N1 –C1	113.2(4)
N1 –C5	1.469(7)	C6 –N1 –C1	122.7(4)
N1 –C6	1.311(7)	C6 –N1 –C5	124.0(4)
C1 –C2	1.517(8)	C2 –C1 –N1	110.2(4)
C1 –H1A	0.949	H1A –C1 –N1	109.1
C1 –H1B	0.951	H1B –C1 –N1	108.9
C2 –C3	1.518(8)	H1A –C1 –C2	109.8
C2 –H2A	0.954	H1B –C1 –C2	109.4
C2 –H2B	0.944	H1B –C1 –H1A	109.4
C3 –C4	1.531(9)	C3 –C2 –C1	109.3(5)
C3 –H3A	0.945	H2A –C2 –C1	109.2
C3 –H3B	0.952	H2B –C2 –C1	110.0
C4 –C5	1.502(8)	H2A –C2 –C3	108.9
C4 –H4A	0.953	H2B –C2 –C3	109.9
C4 –H4B	0.946	H2B –C2 –H2A	109.6
C5 –H5A	0.950	C4 –C3 –C2	109.8(5)
C5 –H5B	0.950	H3A –C3 –C2	109.9
C6 –C7	1.369(7)	H3B –C3 –C2	109.2
C6 –H6	0.953	H3A –C3 –C4	109.4
C7 –C8	1.384(7)	H3B –C3 –C4	108.8
C7 –H7	0.952	H3B –C3 –H3A	109.8
C8 –C9	1.376(7)	C5 –C4 –C3	110.0(5)
C8 –H8	0.952	H4A –C4 –C3	108.9
C9 –C10	1.381(7)	H4B –C4 –C3	109.6
C9 –H9	0.951	H4A –C4 –C5	109.1
C10 –C11	1.365(7)	H4B –C4 –C5	109.6
C10 –H10	0.952	H4B –C4 –H4A	109.6
C11 –C12	1.428(7)	C4 –C5 –N1	110.8(5)
C11 –C13	1.422(8)	H5A –C5 –N1	109.0
C12 –N2	1.147(7)	H5B –C5 –N1	108.9
C13 –N3	1.131(8)	H5A –C5 –C4	109.4
		H5B –C5 –C4	109.2
		H5B –C5 –H5A	109.5
		C7 –C6 –N1	129.5(5)
		H6 –C6 –N1	115.3
		H6 –C6 –C7	115.2
		C8 –C7 –C6	120.2(5)
		H7 –C7 –C6	119.9
		H7 –C7 –C8	119.9
		C9 –C8 –C7	126.9(5)

Table S3. (Cont.)

			Angle(°)
H8	–C8	–C7	116.4
H8	–C8	–C9	116.7
C10	–C9	–C8	121.6(5)
H9	–C9	–C8	119.1
H9	–C9	–C10	119.3
C11	–C10	–C9	128.3(5)
H10	–C10	–C9	115.8
H10	–C10	–C11	115.9
C12	–C11	–C10	122.3(5)
C13	–C11	–C10	120.9(5)
C13	–C11	–C12	116.8(5)
N2	–C12	–C11	177.9(6)
N3	–C13	–C11	177.6(6)

SUPPLEMENTARY MATERIAL FOR COMPOUND **2**

1,1-dicyano-6-(N-aza-15-crown-5)-1,3,5-hexatriene



J-2526-M12

wps code	aza-15-crown-5 DCV
Name	1,1-dicyano-6-(N-aza-15-crown-5)-1,3,5-hexatriene
Formula	$C_{18}H_{25}N_3O_4$
Formula Weight	347.41
Crystal System	Monoclinic
Space Group	$P2_1/c$, #14
Cell Dimensions a, Å	12.379 (2)
b, Å	15.629 (4)
c, Å	9.700
α, °	90.0
β, °	99.73 (2)
γ, °	90.0
V, Å^3	1849.7 (8)
Z	4
Density, calc, g cm^{-3}	1.248
Crystal color, habit	orange-red, chunky rectangles
Crystal size, mm^3	0.19 x 0.22 x 0.22
μ, cm^{-1}	0.832
μ r_{max}	0.015
maximum 2θ (scan type)	25°
range of h,k, l	-16 - 16, -10 - 10, 0 - 17
# of reflections measured	6974
# of independent reflections	2517
# reflections, $F_o^2 > 0$	2971
# reflections, $F_o^2 > 3\sigma(F_o^2)$	2215
GOF, merge	1.48
R(merge) for refs meas. twice	0.034
secondary extinction (x 10^{-6})	1.48 (10)
R, $F_o^2 > 0$	0.054
R, $F_o^2 > 3\sigma(F_o^2)$	0.0358
GOF (number of parameters)	1.48, (327)
$(\Delta/\sigma)_{max}$ in final least squares	0.03
Final Difference map:	
Maximum, eÅ^{-3}	+ 0.19
Minimum, eÅ^{-3}	- 0.21

Data was collected at 225 K.
Hydrogen atoms were refined isotropically
Structure solved using MULTAN 88.

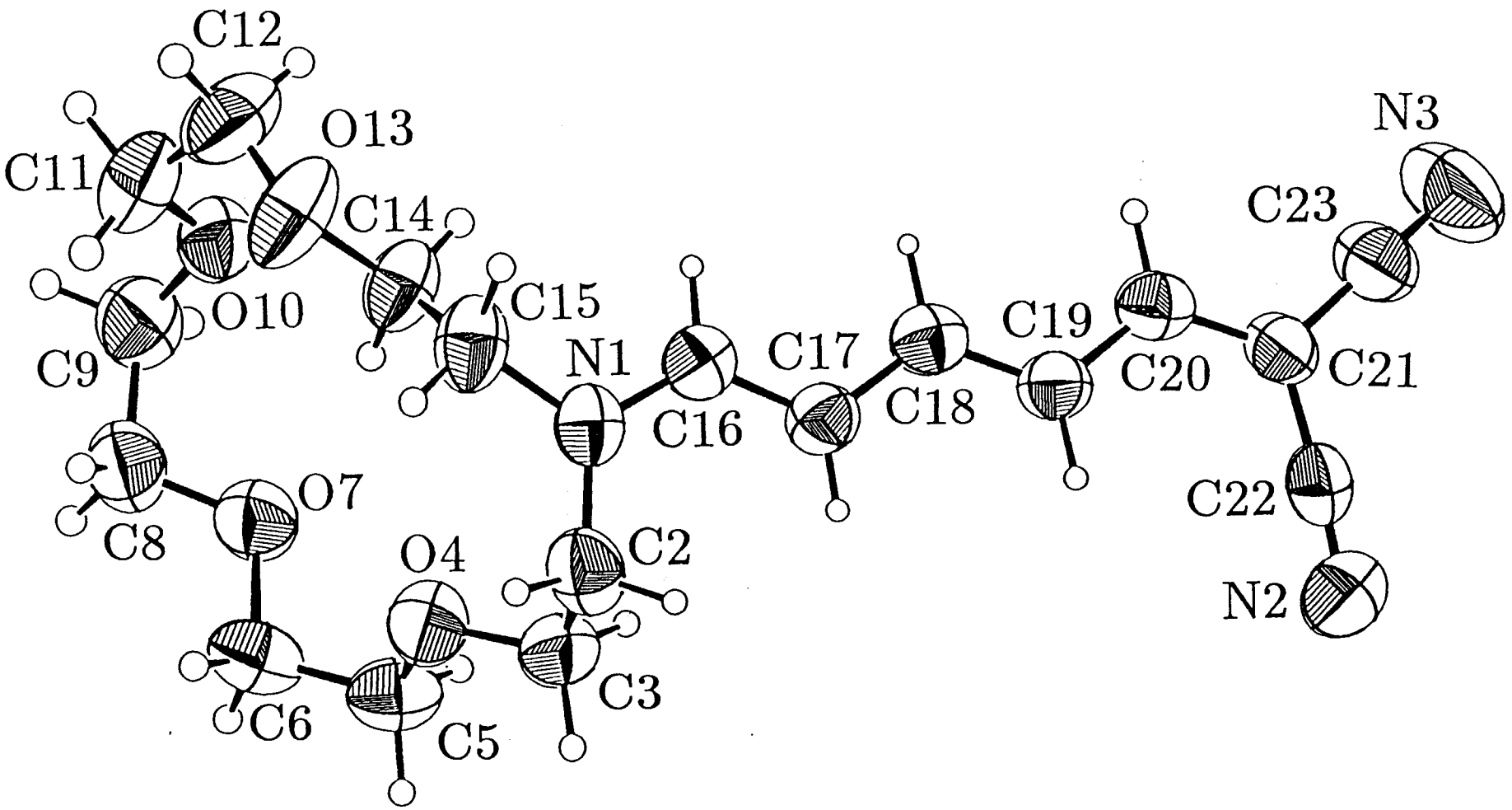


Figure 1: An ORTEP drawing of the molecule with 75% probability elipsoids showing the numbering system. Hydogen atoms are shown with thermal parameters one-tenth of their actual value.

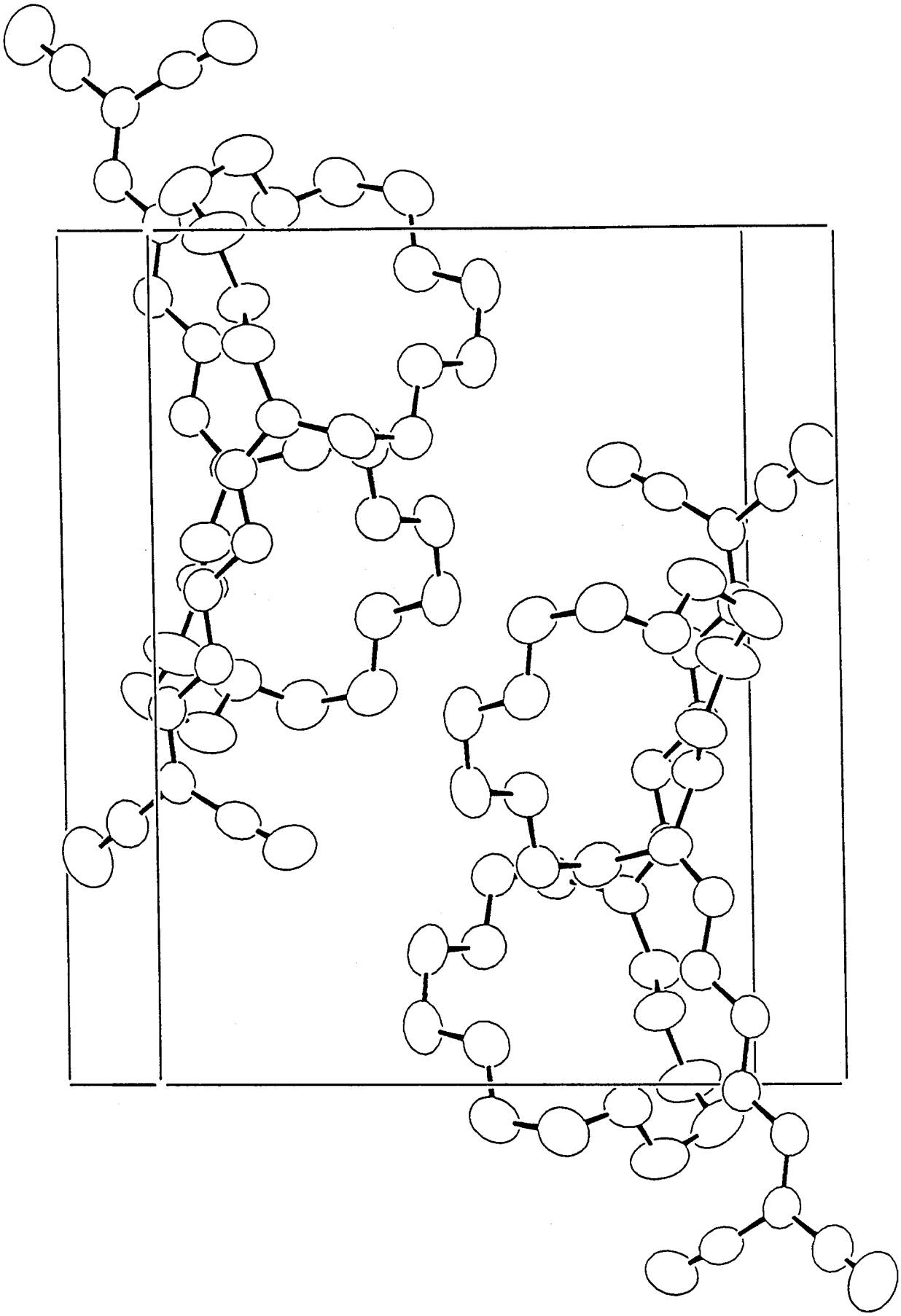


Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Atoms are shown as 75% probability elipsoids; hydogen atoms are not shown The view is perpendicular to the a b plane.

Table 1. Final Refined Parameters for Azo-15-Crown-5-Cyanine.

x, y, z and $U_{eq}{}^{a} \times 10^{4}$

Atom	x	y	z	U_{eq} or B
N1	2403(1)	7783(1)	4137(1)	341(3)
C2	3389(1)	7570(1)	3565(2)	401(4)
C3	4406(2)	7550(1)	4668(2)	394(4)
O4	4630(1)	8389(1)	5173(1)	406(3)
C5	5588(2)	8429(1)	6220(2)	423(5)
C6	5741(2)	9330(1)	6723(2)	431(5)
O7	4919(1)	9528(1)	7528(1)	448(3)
C8	4841(2)	10415(1)	7776(2)	476(5)
C9	3936(2)	10555(1)	8609(2)	489(5)
O10	2905(1)	10260(1)	7900(1)	418(3)
C11	2331(2)	10875(1)	6985(2)	514(5)
C12	1369(2)	10462(1)	6101(3)	579(6)
O13	1631(1)	9962(1)	4991(1)	568(4)
C14	2090(2)	9144(1)	5368(2)	421(5)
C15	1973(2)	8660(1)	4013(2)	420(5)
C16	1860(1)	7187(1)	4720(2)	316(4)
C17	2088(1)	6329(1)	4844(2)	325(4)
C18	1459(1)	5784(1)	5524(2)	318(4)
C19	1618(1)	4921(1)	5690(2)	318(4)
C20	1030(1)	4409(1)	6479(2)	332(4)

Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
C21	1182(1)	3547(1)	6700(2)	340(4)
C22	1987(1)	3103(1)	6087(2)	406(4)
N2	2652(1)	2784(1)	5574(2)	616(5)
C23	567(1)	3065(1)	7542(2)	434(5)
N3	71(1)	2674(1)	8213(2)	670(5)
H2A	3300(12)	6990(10)	3120(16)	2.8(4)*
H2B	3481(13)	7997(11)	2876(18)	3.4(4)*
H3A	4299(13)	7147(10)	5469(18)	3.2(4)*
H3B	5019(13)	7315(10)	4263(17)	3.3(4)*
H5A	5486(13)	8032(10)	7016(19)	3.6(4)*
H5B	6224(14)	8230(10)	5835(17)	3.3(4)*
H6A	6477(14)	9362(10)	7315(18)	3.8(4)*
H6B	5694(14)	9728(11)	5921(19)	4.1(4)*
H8A	5563(15)	10634(11)	8344(19)	4.4(4)*
H8B	4672(14)	10735(11)	6886(20)	4.1(4)*
H9A	4117(15)	10214(12)	9504(20)	4.9(5)*
H9B	3904(14)	11196(12)	8830(18)	4.3(4)*
H11A	2050(14)	11354(12)	7542(20)	4.8(5)*
H11B	2811(16)	11109(12)	6382(22)	5.8(6)*
H12A	970(14)	10113(12)	6704(20)	4.4(5)*

Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
H12B	895(16)	10923(13)	5659(21)	5.6(5)*
H14A	2848(15)	9193(10)	5800(18)	3.9(4)*
H14B	1669(14)	8856(11)	6033(19)	4.1(4)*
H15A	1169(15)	8628(10)	3570(18)	3.8(4)*
H15B	2352(14)	8957(11)	3348(19)	4.1(4)*
H16	1237(12)	7383(9)	5106(16)	2.4(3)*
H17	2673(12)	6095(9)	4480(16)	2.4(3)*
H18	874(12)	6059(9)	5926(15)	1.9(3)*
H19	2168(12)	4649(9)	5248(16)	2.6(3)*
H20	472(13)	4676(10)	6935(16)	3.1(4)*

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

Table 2. Anisotropic Dispalcement Parameters for Azo-15-Crown-5-Cyanine.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N1	380(8)	302(8)	334(8)	−22(6)	36(7)	21(6)
C2	487(11)	402(11)	340(11)	−77(9)	144(9)	−25(9)
C3	400(10)	381(10)	426(12)	28(9)	145(9)	−14(9)
O4	384(7)	402(7)	409(7)	11(5)	−3(6)	−2(6)
C5	317(10)	549(12)	394(11)	66(9)	36(9)	−20(10)
C6	304(10)	589(13)	403(11)	−37(9)	69(9)	−29(10)
O7	467(7)	437(8)	477(8)	−44(6)	185(6)	−42(6)
C8	526(13)	433(12)	491(13)	−103(9)	151(11)	−57(10)
C9	534(12)	493(13)	455(12)	−75(10)	123(10)	−102(10)
O10	465(7)	351(6)	452(8)	−8(6)	121(6)	35(6)
C11	684(14)	343(11)	518(13)	81(10)	108(12)	7(10)
C12	546(13)	483(13)	695(16)	199(11)	66(12)	−35(12)
O13	761(9)	362(7)	535(9)	180(7)	−23(7)	−1(6)
C14	490(12)	317(10)	429(12)	73(9)	1(10)	20(9)
C15	497(12)	322(10)	408(12)	2(9)	−20(10)	57(9)
C16	315(9)	332(10)	291(10)	−1(8)	20(8)	−22(7)
C17	318(9)	322(10)	338(10)	6(8)	63(8)	−33(8)
C18	284(9)	362(10)	298(9)	11(7)	23(8)	−34(8)
C19	291(9)	337(10)	333(10)	5(7)	73(8)	−23(8)
C20	276(9)	381(10)	340(10)	7(7)	51(8)	−21(8)
C21	284(9)	362(10)	381(10)	−27(7)	79(8)	41(8)
C22	406(11)	291(9)	534(12)	−41(8)	117(9)	70(9)
N2	631(11)	403(10)	894(14)	82(8)	363(11)	56(9)
C23	334(10)	460(11)	511(12)	−13(8)	76(9)	95(9)
N3	533(10)	744(13)	771(13)	−82(9)	216(10)	279(11)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table 3. Complete Distances and Angles for Azo-15-Crown-5-Cyanine.

	Distance(Å)		Distance(Å)
N1 –C2	1.463(2)	C18 –C19	1.369(2)
N1 –C15	1.469(2)	C18 –H18	0.978(14)
N1 –C16	1.330(2)	C19 –C20	1.394(2)
C2 –C3	1.508(3)	C19 –H19	0.962(15)
C2 –H2A	1.002(16)	C20 –C21	1.372(2)
C2 –H2B	0.964(17)	C20 –H20	0.976(15)
C3 –O4	1.411(2)	C21 –C22	1.424(2)
C3 –H3A	1.026(16)	C21 –C23	1.422(2)
C3 –H3B	0.983(16)	C22 –N2	1.146(2)
O4 –C5	1.426(2)	C23 –N3	1.144(3)
C5 –C6	1.492(3)		
C5 –H5A	1.016(17)		
C5 –H5B	0.978(16)		
C6 –O7	1.419(2)		
C6 –H6A	0.993(17)		
C6 –H6B	0.990(17)		
O7 –C8	1.413(2)		
C8 –C9	1.503(3)		
C8 –H8A	1.026(18)		
C8 –H8B	0.989(18)		
C9 –O10	1.421(2)		
C9 –H9A	1.011(19)		
C9 –H9B	1.026(18)		
O10 –C11	1.416(2)		
C11 –C12	1.491(3)		
C11 –H11A	1.018(18)		
C11 –H11B	0.97(2)		
C12 –O13	1.412(3)		
C12 –H12A	0.990(18)		
C12 –H12B	0.98(2)		
O13 –C14	1.421(2)		
C14 –C15	1.502(3)		
C14 –H14A	0.963(17)		
C14 –H14B	1.002(17)		
C15 –H15A	1.017(17)		
C15 –H15B	0.976(18)		
C16 –C17	1.370(2)		
C16 –H16	0.963(15)		
C17 –C18	1.394(2)		
C17 –H17	0.932(15)		

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Table 3. (Cont.)

	Angle(°)		Angle(°)
C15 –N1 –C2	119.7(1)	H9B –C9 –H9A	110.2(14)
C16 –N1 –C2	121.1(1)	C11 –O10 –C9	113.4(1)
C16 –N1 –C15	119.2(1)	C12 –C11 –O10	109.5(2)
C3 –C2 –N1	112.7(1)	H11A –C11 –O10	110.3(10)
H2A –C2 –N1	109.3(9)	H11B –C11 –O10	109.8(12)
H2B –C2 –N1	108.0(10)	H11A –C11 –C12	108.2(10)
H2A –C2 –C3	107.8(9)	H11B –C11 –C12	109.1(12)
H2B –C2 –C3	108.9(10)	H11B –C11 –H11A	109.9(16)
H2B –C2 –H2A	110.2(13)	O13 –C12 –C11	114.5(2)
O4 –C3 –C2	108.6(1)	H12A –C12 –C11	109.1(11)
H3A –C3 –C2	110.6(9)	H12B –C12 –C11	107.1(12)
H3B –C3 –C2	109.4(9)	H12A –C12 –O13	110.3(11)
H3A –C3 –O4	110.6(9)	H12B –C12 –O13	105.7(12)
H3B –C3 –O4	111.5(9)	H12B –C12 –H12A	110.0(16)
H3B –C3 –H3A	106.3(13)	C14 –O13 –C12	115.8(1)
C5 –O4 –C3	112.3(1)	C15 –C14 –O13	104.6(1)
C6 –C5 –O4	108.5(1)	H14A –C14 –O13	111.0(10)
H5A –C5 –O4	108.6(10)	H14B –C14 –O13	109.9(10)
H5B –C5 –O4	109.9(10)	H14A –C14 –C15	111.3(10)
H5A –C5 –C6	110.7(10)	H14B –C14 –C15	110.7(10)
H5B –C5 –C6	111.1(10)	H14B –C14 –H14A	109.3(14)
H5B –C5 –H5A	107.9(13)	C14 –C15 –N1	114.7(2)
O7 –C6 –C5	108.8(1)	H15A –C15 –N1	107.7(10)
H6A –C6 –C5	106.8(10)	H15B –C15 –N1	106.8(10)
H6B –C6 –C5	110.4(10)	H15A –C15 –C14	109.8(10)
H6A –C6 –O7	110.1(10)	H15B –C15 –C14	110.7(10)
H6B –C6 –O7	110.1(10)	H15B –C15 –H15A	106.8(14)
H6B –C6 –H6A	110.5(14)	C17 –C16 –N1	127.7(2)
C8 –O7 –C6	112.6(1)	H16 –C16 –N1	115.9(9)
C9 –C8 –O7	108.2(2)	H16 –C16 –C17	116.4(9)
H8A –C8 –O7	109.9(10)	C18 –C17 –C16	121.1(1)
H8B –C8 –O7	110.9(10)	H17 –C17 –C16	120.8(9)
H8A –C8 –C9	108.8(10)	H17 –C17 –C18	118.1(9)
H8B –C8 –C9	109.2(10)	C19 –C18 –C17	125.2(2)
H8B –C8 –H8A	109.7(14)	H18 –C18 –C17	115.5(8)
O10 –C9 –C8	112.5(2)	H18 –C18 –C19	119.3(8)
H9A –C9 –C8	107.9(11)	C20 –C19 –C18	123.5(2)
H9B –C9 –C8	108.3(10)	H19 –C19 –C18	118.8(9)
H9A –C9 –O10	107.1(11)	H19 –C19 –C20	117.8(9)
H9B –C9 –O10	110.8(10)	C21 –C20 –C19	125.4(2)

Table 3. (Cont.)

			Angle(°)
H20	–C20	–C19	118.6(9)
H20	–C20	–C21	116.0(9)
C22	–C21	–C20	119.9(1)
C23	–C21	–C20	122.5(2)
C23	–C21	–C22	117.6(1)
N2	–C22	–C21	176.7(2)
N3	–C23	–C21	179.6(2)

Table 4. Intermolecular Distances Less Than 3.5 Å for Azo-15-Crown-5-Cyanine.

	Distance(Å)		Distance(Å)
C2 –H3A	3.409(16)	C17 –H15B	3.389(17)
C2 –H5A	3.346(17)	C17 –H8A	3.316(18)
C3 –H5A	3.225(17)	C18 –H15A	3.171(17)
C3 –H8B	3.369(18)	C18 –H15B	2.805(17)
C3 –H9B	3.154(17)	C18 –C20	3.366(2)
O4 –H6B	3.130(17)	C18 –H20	3.161(15)
O4 –H8B	2.682(18)	C19 –H15B	3.124(17)
C5 –H3B	3.357(16)	C19 –H9A	3.484(19)
C5 –H8B	3.250(18)	C19 –H20	3.369(15)
C6 –H6B	3.218(17)	C19 –H6A	2.920(17)
C6 –H8B	3.453(18)	C20 –H15B	3.390(17)
O7 –H2A	3.219(15)	C20 –H18	3.110(14)
O7 –H3B	3.327(16)	C20 –H12A	3.454(18)
O7 –H9A	2.952(19)	C20 –H6A	3.111(17)
C8 –H2B	3.365(17)	C21 –H18	3.340(14)
C8 –H9A	2.905(19)	C21 –H6A	3.162(17)
C8 –H3A	3.279(16)	C22 –H11A	3.072(18)
C9 –H17	3.203(15)	C22 –H11B	3.28(2)
C9 –H19	2.931(15)	C22 –H5A	3.353(17)
C9 –H8A	3.457(18)	C22 –H5B	3.409(16)
C9 –H9A	3.019(19)	C22 –H6A	2.982(17)
C9 –H3A	3.332(16)	N2 –H11A	3.111(18)
O10 –C17	3.375(2)	N2 –H11B	2.73(2)
O10 –C19	3.375(2)	N2 –H9B	2.948(17)
O10 –H17	2.658(15)	N2 –H11A	3.206(18)
O10 –H19	2.595(15)	N2 –H3B	2.865(16)
C11 –N2	3.334(3)	N2 –H5B	2.637(16)
C11 –H19	3.308(15)	N2 –H5A	3.018(17)
C12 –H20	3.434(15)	N2 –H6A	3.270(17)
O13 –H20	3.119(15)	C23 –H11A	3.244(18)
O13 –H12A	3.361(18)	C23 –H12B	3.37(2)
O13 –H12B	3.38(2)	C23 –H15A	3.464(17)
C14 –H2A	3.340(16)	C23 –H16	3.183(15)
C15 –C18	3.447(2)	N3 –H11A	3.350(18)
C15 –H18	3.104(14)	N3 –H12B	3.26(2)
C16 –H2B	3.377(17)	N3 –H15A	2.931(17)
C16 –C23	3.431(2)	N3 –H16	3.351(15)
C16 –N3	3.400(2)	N3 –H14B	3.019(17)
C16 –N3	3.454(2)	N3 –H16	2.526(15)
C17 –H2B	3.320(17)	N3 –H18	2.961(14)

Table 4. (Cont.)

	Distance(Å)		Distance(Å)
H2A –H3A	3.32(2)	H12B –H15A	2.87(3)
H2A –H5A	3.07(2)	H14B –H17	3.37(2)
H2A –H14A	2.89(2)	H15A –H18	2.58(2)
H2A –H14B	2.92(2)	H15A –H20	3.13(2)
H2B –H3A	2.71(2)	H15B –H18	2.72(2)
H2B –H5A	3.18(2)	H15B –H20	3.28(2)
H2B –H8A	2.80(2)	H18 –H20	3.20(2)
H2B –H8B	3.01(2)		
H3A –H8A	2.62(2)		
H3A –H8B	3.46(2)		
H3A –H9B	2.67(2)		
H3B –H5A	2.41(2)		
H3B –H8B	3.29(2)		
H3B –H9B	2.72(2)		
H5A –H9B	3.11(2)		
H5B –H8B	3.13(2)		
H5B –H11B	2.83(3)		
H5B –H9B	3.20(2)		
H6A –H15B	3.12(2)		
H6A –H9A	3.36(3)		
H6A –H19	2.70(2)		
H6B –H6B	2.41(2)		
H6B –H8B	2.78(3)		
H6B –H11B	3.39(3)		
H6B –H14A	3.15(2)		
H6B –H15B	3.16(3)		
H8A –H15B	3.35(3)		
H8A –H9A	2.45(3)		
H8A –H17	2.86(2)		
H8A –H19	3.29(2)		
H9A –H17	2.71(2)		
H9A –H19	2.64(2)		
H9A –H9A	2.33(3)		
H9A –H9B	3.48(3)		
H9B –H19	3.04(2)		
H11A –H19	3.04(2)		
H12A –H12B	3.38(3)		
H12A –H15A	3.27(3)		
H12A –H20	2.49(2)		
H12B –H14B	3.34(3)		

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Scattering Factors and f', f'':

Cromer, D. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 149–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Cromer, D. T. & Waber, J. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Any additional Data:

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data were obtained by propagation of error plus another additional term, $(0.014\bar{I})^2$.

Definitions:

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma F_o}; \quad R_w = \frac{\Sigma w(F_o^2 - F_c^2)}{\Sigma w F_o^2}$$

$$S = \left\{ \frac{\Sigma w(F_o^2 - F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}$$

where n = number of data,

p = number of parameters refined.

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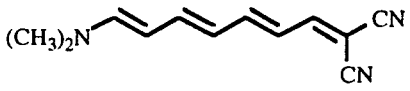
J-2526-M25

JA933907

SUPPLEMENTARY MATERIAL FOR COMPOUND 4

1,1-dicyano-8-(dimethylamino)-octa-1,3,5,7-tetraene



wps code	Me2N-III-DCV
Name	1,1-dicyano-8-(dimethylamino)-octa-1,3,5,7-tetraene
Formula	$C_{12}H_{13}N_3$
Formula Weight	199.25
Crystal System	Monoclinic
Space Group	$P2_1/c$, #14
Cell Dimensions a, Å	9.242 (6)
b, Å	16.096 (7)
c, Å	8.188 (3)
α, °	90.0
β, °	105.38 (4)
γ, °	90.0
V, $Å^3$	1174.4 (0)
Z	4
Density, calc, g cm^{-3}	1.13
Crystal color, habit	dark, wide blade
Crystal size, mm^3	0.19 x 0.36 x 0.70
μ, cm^{-1}	0.65
μr_{max}	0.455
maximum 2θ (scan type)	25°
range of h, k, l	-9 - 9, -19 - 19, 0 - 11
# of reflections measured	4672
# of independent reflections	2060
# reflections, $F_o^2 > 0$	1797
# reflections, $F_o^2 > 3\sigma(F_o^2)$	1390
GOF, merge	1.02
R(merge) for refs meas. twice	0.025
secondary extinction (x 10^{-6})	1.9 (4)
R, $F_o^2 > 0$	0.065
R, $F_o^2 > 3\sigma(F_o^2)$	0.051
GOF (number of parameters)	2.66, (137)
$(\Delta/\sigma)_{max}$ in final least squares	0.02
Final Difference map:	
Maximum, $eÅ^{-3}$	+ 0.21
Minimum, $eÅ^{-3}$	- 0.19

Data was collected at 225 K.
Hydrogen atoms were refined isotropically
Structure solved using MULTAN 88.

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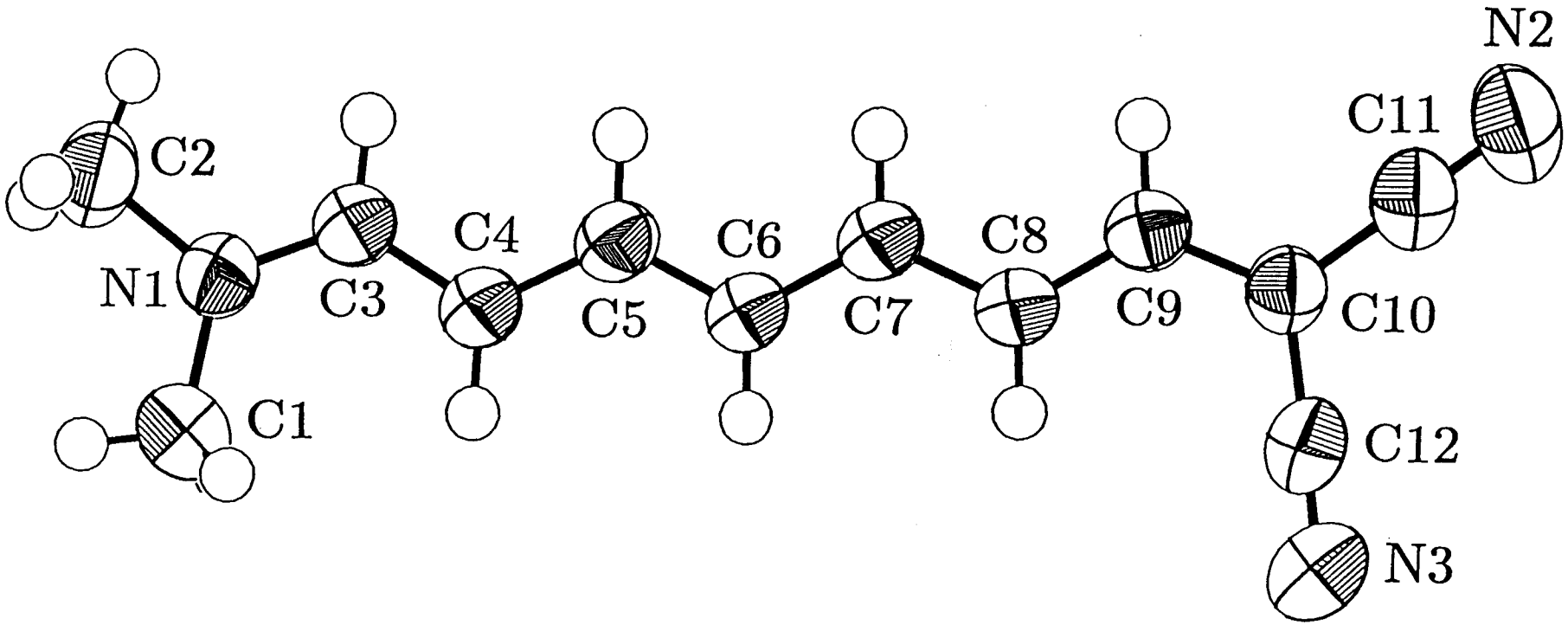

Figure 1: An ORTEP drawing of the molecule with 50% probability elipsoids showing the numbering system. Hydogen atoms are shown as spheres of of small, srbitrary size.

J-2526-M28

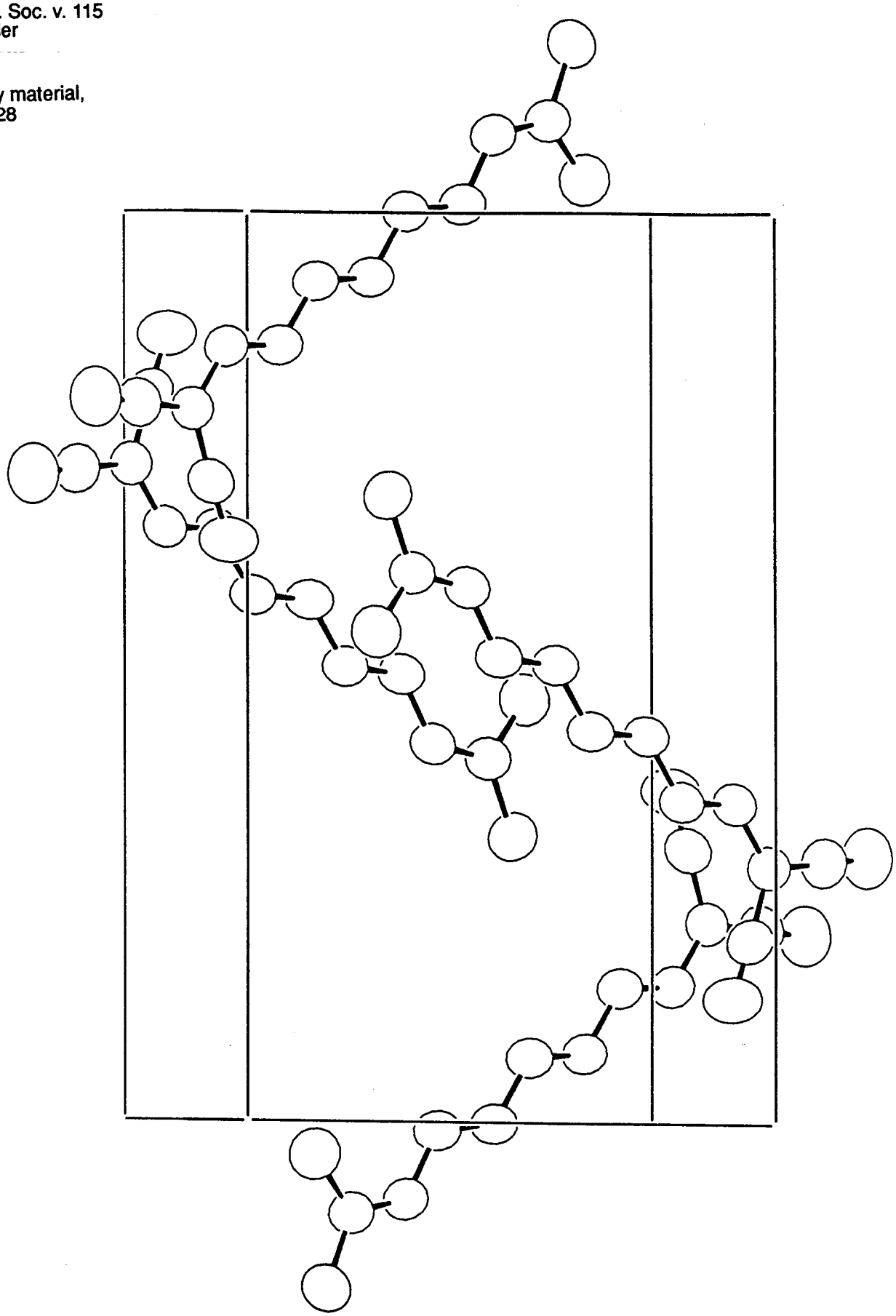

Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Atoms are shown as 50% probability elipsoids; Hydrogen atoms are not shown.

J-2526-m29

Table 1. Final Refined Parameters for 2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
C1	7476(3)	367(2)	4559(3)	863(6)
C2	7098(3)	1864(1)	3920(3)	842(6)
N1	6555(2)	1015(1)	3588(2)	668(4)
C3	5258(2)	858(1)	2499(2)	633(5)
C4	4574(2)	96(1)	2126(2)	638(5)
C5	3216(2)	15(1)	924(2)	629(5)
C6	2436(2)	−712(1)	456(2)	642(5)
C7	1092(2)	−761(1)	−788(2)	619(5)
C8	292(2)	−1477(1)	−1341(2)	614(5)
C9	−1012(2)	−1498(1)	−2636(2)	615(5)
C10	−1820(2)	−2191(1)	−3319(2)	630(5)
C11	−3158(3)	−2130(1)	−4650(3)	745(6)
N2	−4234(2)	−2071(1)	−5728(3)	1013(6)
C12	−1325(2)	−2999(1)	−2733(3)	705(6)
N3	−883(2)	−3640(1)	−2245(3)	971(7)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table 2. Assigned Hydrogen Atom Parameters for 2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

x, y and $z \times 10^4$

Atom	x	y	z	B
H1 A	8353	610	5262	7.0
H1 B	7725	−17	3793	7.0
H1 C	6915	96	5222	7.0
H2 A	7973	1924	3527	7.0
H2 B	7324	1961	5099	7.0
H2 C	6334	2230	3325	7.0
H3	4730	1321	1903	6.0
H4	5051	−385	2708	6.0
H5	2778	509	367	6.0
H6	2844	−1209	1017	6.0
H7	676	−254	−1308	6.0
H8	668	−1985	−797	6.0
H9	−1398	−976	−3108	6.0

Table 3. Anisotropic Displacement Parameters for 2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	749(15)	897(16)	865(15)	40(13)	78(12)	40(13)
C2	729(15)	760(14)	1008(17)	−111(12)	180(13)	−171(13)
N1	628(11)	593(10)	738(11)	−1(8)	101(9)	−74(8)
C3	640(13)	571(12)	660(12)	31(10)	125(11)	−37(10)
C4	681(13)	540(12)	658(12)	24(10)	115(11)	−29(9)
C5	695(13)	535(11)	650(12)	12(10)	164(11)	−25(9)
C6	694(13)	516(11)	684(13)	17(10)	127(11)	−6(9)
C7	666(13)	522(11)	664(12)	26(10)	170(11)	−18(9)
C8	636(13)	531(11)	650(12)	34(10)	126(11)	13(9)
C9	634(13)	572(12)	649(12)	40(10)	190(11)	7(10)
C10	578(13)	631(13)	678(13)	−23(10)	163(11)	−65(10)
C11	664(15)	798(16)	776(15)	−64(12)	198(13)	−127(12)
N2	723(13)	1210(17)	998(15)	−60(12)	37(12)	−185(13)
C12	715(14)	671(15)	733(14)	−102(12)	200(11)	−115(12)
N3	1094(17)	666(13)	1110(16)	−42(12)	215(13)	−56(12)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table 4. Complete Distances and Angles for 2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

	Distance(Å)				Angle(°)
C1 –N1	1.446(3)	C2	–N1	–C1	116.8(2)
C2 –N1	1.455(3)	C3	–N1	–C1	122.1(2)
N1 –C3	1.315(2)	C3	–N1	–C2	121.0(2)
C3 –C4	1.376(3)	C4	–C3	–N1	127.2(2)
C4 –C5	1.380(3)	C5	–C4	–C3	121.3(2)
C5 –C6	1.374(3)	C6	–C5	–C4	126.2(2)
C6 –C7	1.383(3)	C7	–C6	–C5	123.8(2)
C7 –C8	1.379(3)	C8	–C7	–C6	126.0(2)
C8 –C9	1.378(3)	C9	–C8	–C7	123.8(2)
C9 –C10	1.375(3)	C10	–C9	–C8	127.1(2)
C10 –C11	1.419(3)	C11	–C10	–C9	121.7(2)
C10 –C12	1.420(3)	C12	–C10	–C9	120.9(2)
C11 –N2	1.145(3)	C12	–C10	–C11	117.4(2)
C12 –N3	1.142(3)	N2	–C11	–C10	179.1(2)
C1 –H1 A	0.946	N3	–C12	–C10	177.9(2)
C1 –H1 B	0.951	H1 A	–C1	–N1	108.7
C1 –H1 C	0.951	H1 B	–C1	–N1	108.4
C2 –H2 A	0.951	H1 C	–C1	–N1	108.3
C2 –H2 B	0.945	H1 B	–C1	–H1 A	110.6
C2 –H2 C	0.949	H1 C	–C1	–H1 A	110.7
C3 –H3	0.952	H1 C	–C1	–H1 B	110.1
C4 –H4	0.953	H2 A	–C2	–N1	108.3
C5 –H5	0.953	H2 B	–C2	–N1	108.5
C6 –H6	0.950	H2 C	–C2	–N1	108.3
C7 –H7	0.953	H2 B	–C2	–H2 A	110.6
C8 –H8	0.952	H2 C	–C2	–H2 A	110.3
C9 –H9	0.953	H2 C	–C2	–H2 B	110.8
		H3	–C3	–N1	116.6
		H3	–C3	–C4	116.2
		H4	–C4	–C3	119.2
		H4	–C4	–C5	119.5
		H5	–C5	–C4	116.9
		H5	–C5	–C6	116.9
		H6	–C6	–C5	118.0
		H6	–C6	–C7	118.2
		H7	–C7	–C6	117.2
		H7	–C7	–C8	116.8
		H8	–C8	–C7	117.8
		H8	–C8	–C9	118.3
		H9	–C9	–C8	116.5
		H9	–C9	–C10	116.4

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Table 5. Intermolecular Distances Less Than 3.5 Åfor 2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

		Distance(Å)			Distance(Å)
C1	–H9	2.889	H1 C	–H9	2.480
C2	–N2	3.375(3)	H1 C	–H1 C	3.474
C2	–H6	3.103	H1 C	–H4	2.832
C2	–H8	2.894	H2 A	–H2 B	3.251
C3	–H1 C	3.443	H2 A	–H8	2.842
C4	–H1 C	2.879	H2 A	–H6	3.145
C5	–H9	3.164	H2 A	–H8	2.623
C5	–H1 C	3.194	H2 B	–H2 C	3.285
C6	–H7	3.499	H2 B	–H6	3.444
C7	–H7	3.126	H2 B	–H6	3.076
C7	–H1 B	3.200	H2 B	–H8	2.468
C7	–H2 A	3.211	H2 C	–H6	2.639
C8	–H2 A	2.795	H2 C	–H8	3.224
C8	–H2 B	3.321	H5	–H9	2.958
C9	–H1 C	3.398	H7	–H7	2.871
C9	–H5	3.203			
C9	–H2 A	3.159			
C10	–H3	3.492			
C11	–C12	3.399(3)			
C11	–H2 C	3.392			
C11	–H3	3.256			
C11	–H3	3.210			
N2	–H4	2.999			
N2	–H2 B	3.038			
N2	–H2 C	3.120			
N2	–H3	3.499			
N2	–H2 C	2.714			
N2	–H3	2.757			
C12	–H8	3.484			
C12	–H5	3.268			
N3	–H1 B	2.762			
N3	–H5	3.017			
N3	–H7	2.882			
N3	–H1 A	2.747			
N3	–H2 B	3.432			
H1 A	–H7	3.352			
H1 A	–H9	2.862			
H1 B	–H9	2.897			
H1 B	–H5	3.406			
H1 B	–H7	2.847			

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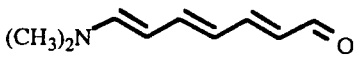
SUPPLEMENTARY MATERIAL FOR COMPOUND **5**

7-dimethylamino-hepta-2,4,6-triene-1-al



wps code	Me2N-III-CHO
Name	7-dimethylamino-hepta-2,4,6-triene-1-al
Formula	$C_9H_{13}NO$
Formula Weight	151.21
Crystal System	Orthorhombic
Space Group	Pbca, #61
Cell Dimensions a, Å	8.189 (3)
b, Å	7.558 (2)
c, Å	28.295 (12)
α, °	90.0
β, °	90.0
γ, °	90.0
V, Å^3	1751.2 (12)
Z	8
Density, calc, g cm^{-3}	1.147
Crystal color, habit	orange plate
Crystal size, mm^3	0.03 x 0.67 x 0.73
μ, cm^{-1}	0.70
μ r_{max}	0.511
maximum 2θ (scan type)	25°
range of h, k, l	0-9, 0-9, -33-33
# of reflections measured	3680
# of independent reflections	1545
# reflections, $F_o^2 > 0$	1370
# reflections, $F_o^2 > 3\sigma(F_o^2)$	904
GOF, merge	0.937
R(merge) for refs meas. twice	0.038
secondary extinction (x 10^{-6})	0.32(6)
R, $F_o^2 > 0$	0.063
R, $F_o^2 > 3\sigma (F_o^2)$	0.035
GOF (number of parameters)	1.44, (153)
$(\Delta/\sigma)_{max}$ in final least squares	0.01
Final Difference map:	
Maximum, eÅ^{-3}	+ 0.21
Minimum, eÅ^{-3}	- 0.23

Data was collected at 225 K.
Hydrogen atoms were refined isotropically
Structure solved using MULTAN 88.

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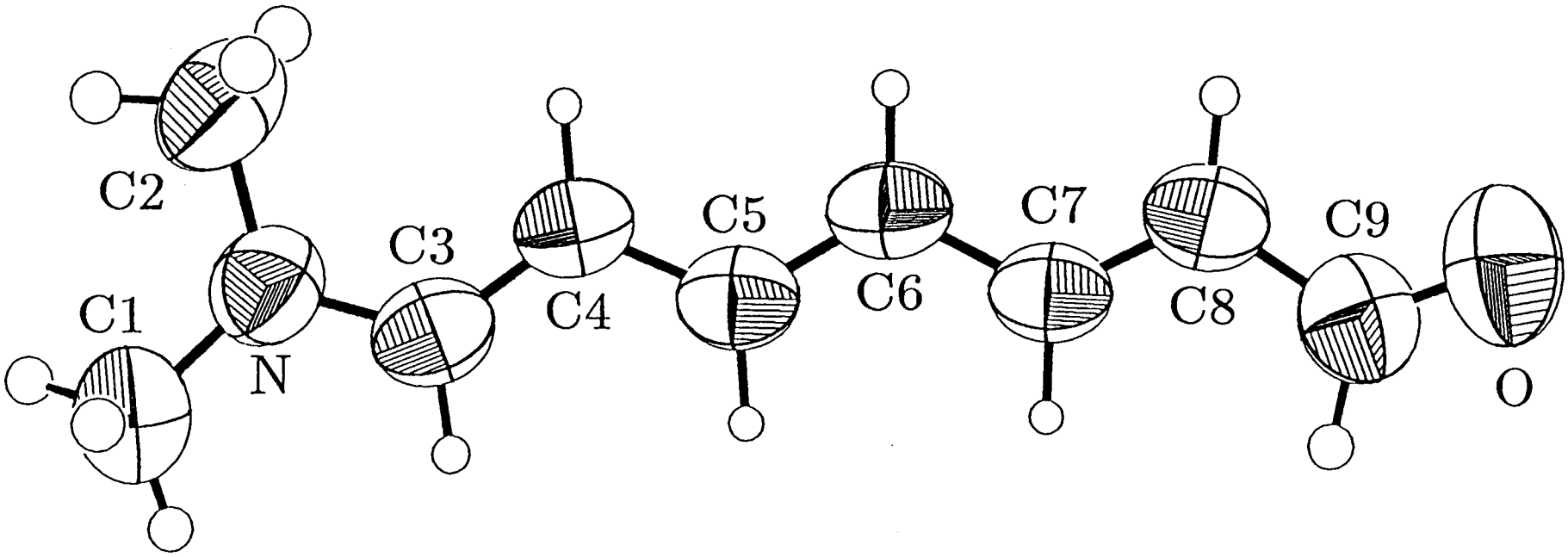

Figure 1: An ORTEP drawing of the molecule with 80% probability elipsoids showing the numbering system. Hydrogen atoms are shown as one tenth actual size.

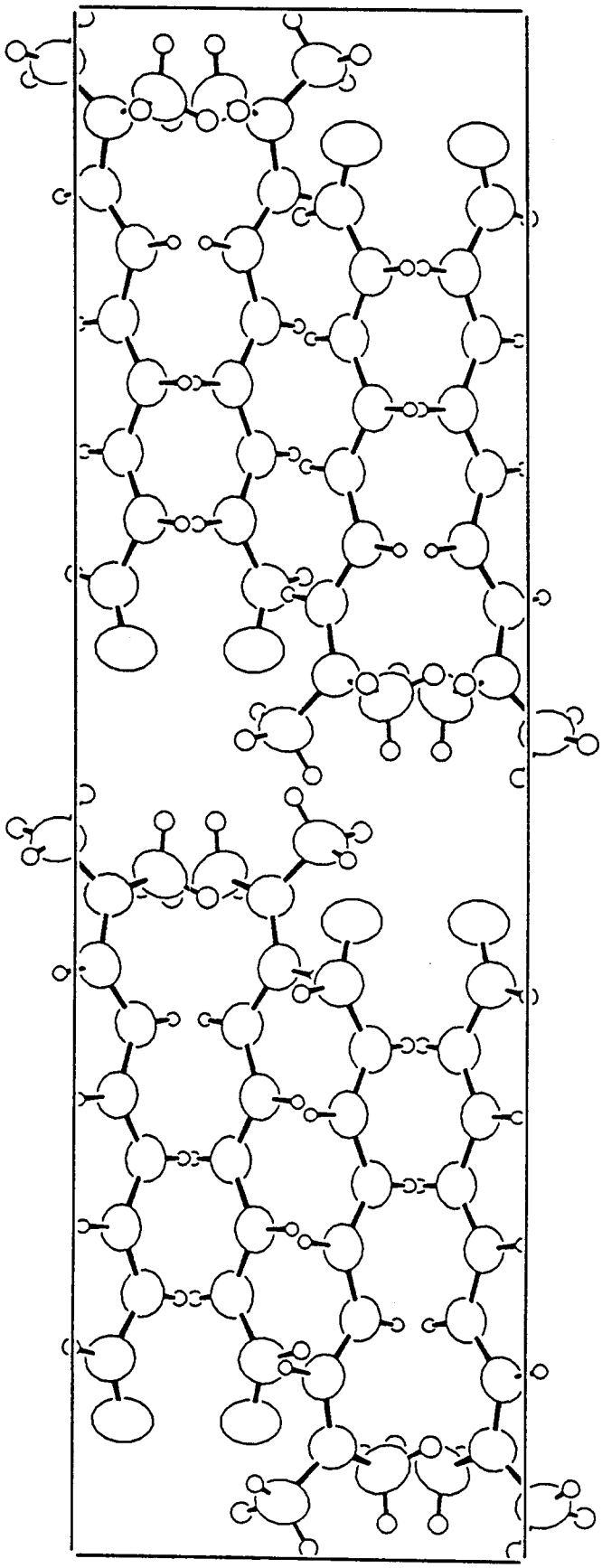

Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Atoms are shown as 70% probability elipsoids; hydrogen atoms are shown at one-tenth actual size.

Table 1. Final Refined Parameters for $Me_2N - III - CHO$.

x, y, z and $U_{eq}{}^a \times 10^4$

Atom	x	y	z	U_{eq} or B
C1	10387(3)	2798(3)	364(1)	594(6)
C2	8157(3)	736(3)	581(1)	571(6)
N	9277(2)	2129(2)	719	452(4)
C3	9479(2)	2553(3)	1174(1)	410(4)
C4	8673(2)	1886(2)	1556(1)	391(4)
C5	9068(2)	2443(3)	2017(1)	390(4)
C6	8438(2)	1812(2)	2427(1)	389(4)
C7	8971(2)	2394(2)	2876(1)	382(4)
C8	8484(2)	1790(3)	3301(1)	418(5)
C9	9182(2)	2469(3)	3726(1)	493(5)
O	8912(2)	1955(2)	4127	683(4)
HC1a	10997(21)	3786(25)	476(6)	5.0(5)*
HC1b	11296(24)	1876(29)	292(6)	7.4(6)*
HC1c	9795(25)	3015(24)	69(7)	5.8(5)*
HC2a	7104(30)	915(29)	730(7)	8.0(7)*
HC2b	8585(26)	−387(30)	666(7)	8.0(7)*
HC2c	8068(22)	768(26)	235(7)	6.7(6)*
HC3	10325(18)	3397(21)	1232(5)	3.6(4)*
HC4	7856(18)	1029(20)	1519(4)	3.1(4)*
HC5	9914(19)	3340(20)	2048(5)	3.2(4)*

Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
HC6	7619(21)	952(20)	2421(5)	3.3(4)*
HC7	9798(18)	3304(20)	2871(5)	3.0(4)*
HC8	7677(20)	914(23)	3330(5)	3.8(4)*
HC9	10025(21)	3421(23)	3656(6)	5.2(5)*

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

Table 2. Anisotropic Displacement Parameters for $Me_2N - III - CHO$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	676(14)	652(16)	453(12)	−60(14)	38(11)	−11(11)
C2	655(15)	522(14)	535(14)	−25(13)	−128(12)	−86(11)
N	507(9)	421(9)	427(8)	−2(8)	−22(7)	−40(7)
C3	402(10)	342(10)	487(11)	8(10)	−38(9)	−32(9)
C4	366(10)	329(11)	479(11)	−26(9)	−30(8)	−21(9)
C5	363(9)	302(11)	505(11)	14(10)	12(8)	−18(9)
C6	354(9)	309(10)	504(12)	−28(9)	5(9)	−24(9)
C7	345(9)	294(10)	506(11)	−3(9)	9(9)	−2(9)
C8	399(11)	342(11)	512(12)	−2(10)	14(9)	34(9)
C9	537(11)	449(12)	494(11)	51(11)	19(10)	31(10)
O	828(10)	759(10)	463(8)	52(9)	−14(7)	110(7)

$U_{i,j}$ values have been multiplied by 10^4
The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table 3. Complete Distances and Angles for $Me_2N - III - CHO$.

	Distance(Å)		Angle(°)
C1 –N	1.446(3)	HC1a –C1 –N	111.8(11)
C1 –HC1a	0.953(18)	HC1b –C1 –N	110.6(11)
C1 –HC1b	1.04(2)	HC1c –C1 –N	109.8(12)
C1 –HC1c	0.98(2)	HC1b –C1 –HC1a	102.4(15)
C2 –N	1.450(3)	HC1c –C1 –HC1a	114.4(16)
C2 –HC2a	0.97(2)	HC1c –C1 –HC1b	107.5(16)
C2 –HC2b	0.95(2)	HC2a –C2 –N	110.1(13)
C2 –HC2c	0.979(19)	HC2b –C2 –N	110.3(13)
N –C3	1.338(2)	HC2c –C2 –N	107.3(11)
C3 –C4	1.363(2)	HC2b –C2 –HC2a	110.0(18)
C3 –HC3	0.956(15)	HC2c –C2 –HC2a	111.5(17)
C4 –C5	1.407(2)	HC2c –C2 –HC2b	107.7(17)
C4 –HC4	0.937(14)	C2 –N –C1	117.7(2)
C5 –C6	1.357(2)	C3 –N –C1	120.5(1)
C5 –HC5	0.973(15)	C3 –N –C2	120.8(2)
C6 –C7	1.413(2)	C4 –C3 –N	127.9(2)
C6 –HC6	0.934(15)	HC3 –C3 –N	114.5(9)
C7 –C8	1.347(2)	HC3 –C3 –C4	117.5(9)
C7 –HC7	0.966(14)	C5 –C4 –C3	120.8(2)
C8 –C9	1.427(2)	HC4 –C4 –C3	120.9(9)
C8 –HC8	0.939(16)	HC4 –C4 –C5	118.3(9)
C9 –O	1.219(2)	C6 –C5 –C4	126.8(2)
C9 –HC9	1.017(17)	HC5 –C5 –C4	117.2(9)
		HC5 –C5 –C6	115.9(9)
		C7 –C6 –C5	122.8(2)
		HC6 –C6 –C5	120.2(9)
		HC6 –C6 –C7	117.0(9)
		C8 –C7 –C6	127.3(2)
		HC7 –C7 –C6	115.1(9)
		HC7 –C7 –C8	117.5(9)
		C9 –C8 –C7	120.8(2)
		HC8 –C8 –C7	121.6(10)
		HC8 –C8 –C9	117.6(10)
		O –C9 –C8	126.7(2)
		HC9 –C9 –C8	111.1(10)
		HC9 –C9 –O	122.1(10)

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